Shodh Sari-An International Multidisciplinary Journal

2025, Vol. 04, Issue 02, 193-200
ISSN: 2959-1376
DOI: https://doi.org/10.59231/SARI7818

Study of Anderson localization in disordered system with bond breaking disorder

Malik, Mohammed Zahid
North Carolina State University, US

Abstract

The dynamics and transport of a particle in condensed-matter systems can be described using a tight-binding Hamiltonian. In this work, we present a simple approach to investigate Anderson localization in a three-dimensional system with an off-diagonal disorder. We construct the tight-binding Hamiltonian for the system in which a single random energy is assigned to each lattice site, and the hopping integrals are restricted to nearest-neighbour sites only. We introduce bond-breaking disorder, where some hopping terms between sites are randomly weakened. We compute disorder-impacted density of states (DOS), the inverse participation ratio (IPR), and level statistics to identify the Anderson transition. Emergence of mobility edge has been seen while analysing inverse participation ratio with disorder. We address our problem in the thermodynamic limit by applying appropriate periodic boundary conditions and numerically demonstrate the existence of an Anderson localization transition.

Keywords: Disordered, localization, numerically, inverse participation ratio, dynamic

Introduction

In solid-state physics, Bloch theory serves as a foundational framework for understanding the behaviour of non-interacting electrons in an ideal crystal lattice with a periodic potential. It describes electron states as extended Bloch waves, representing delocalized states distributed throughout the crystal. However, in real-world materials, perfect crystalline order is rarely achieved due to the presence of disorder, randomness, and impurities. This deviation from periodicity renders the crystal potential non-periodic, causing Bloch theory to break down and leading to the confinement of electron states - a phenomenon known as localization. Localization refers to the

@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

concentration of probability amplitude of a particle within a finite region of the solid, profoundly impacting electronic transport properties. A particularly significant manifestation of this phenomenon is Anderson localization (AL), first introduced by P.W. Anderson in 1958 [1]. AL describes the restriction of the wave function of a quantum particle within a disordered medium, resulting in the suppression of diffusion and electronic transport. Over the years, many experimental and theoretical studies [1-8] have carefully studied the complex nature of AL.

Anderson in his pioneering work [1] demonstrated the localization of electron wave functions in a stochastic potential, highlighting the interplay between disorder and electronic behaviour. His study revealed that strong randomness or disorder in the potential leads to an almost complete absence of diffusion. Building on this foundation, Mott [2] extended the concept to electric conduction in random systems, elucidating the underlying dynamics of the metal-insulator (MI) transition driven by increasing impurity concentrations. Further advancements came with the development of the scaling theory of localization by Abrahams, Anderson, Licciardello, and Ramakrishnan [3], which examined the influence of system size on conductance. This theory established that in one-dimensional (1D) and two-dimensional (2D) systems, wave functions are inherently localized regardless of disorder strength.

In contrast, three-dimensional (3D) systems exhibit a critical threshold for disorder strength, beyond which AL occurs. This threshold arises from the increased complexity of spatial arrangements in 3D, allowing for greater interference and scattering effects. Consequently, the concept of mobility edge becomes pivotal in 3D systems. Mobility edge defines the critical energy separating localized states from extended states and plays a significant role in understanding electronic transport.

Notably, the concept of a mobility edge extends beyond 3D systems and has also been explored in lower-dimensional systems as well. In 1980, Aubry and André investigated localization in quasiperiodic potentials and demonstrated the existence of a mobility edge in a 1D system [4]. Their work revealed that the position of the mobility edge depends on the strength of the potential. These findings underscore the richness of the AL phenomenon, which remains an active area of research, driving the development of new theoretical and

@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

experimental approaches that continue to deepen our understanding of this complex field. In this paper, we focus on the phenomenon of AL within a 3D lattice and examine its behaviour under bond-breaking disorder.

Model and Method

The general form of the Anderson Hamiltonian for an electron moving on the d-dimensional lattice of site L^d can be written as:

$$H_{Anderson} = -\sum_{<i,j>} t_{ij}\left[a_i^{\dagger}a_j + H.c.\right] + W\sum_{i} \varepsilon_i\, a_i^{\dagger}a_i \qquad (1)$$

In our specific case, we are dealing with bond breaking disorder, which means that the disorder originates from the hopping term (t_{ij}) being randomly set to zero for a fraction W of the bonds. Since the disorder exclusively affects the hopping amplitudes, the on-site potential term $(\varepsilon_i\, a_i^{\dagger}a_i)$ is not included, and the diagonal elements of the Hamiltonian are zero. Thus, the Hamiltonian simplifies to:

$$H_{Anderson} = -\sum_{<i,j>} \left[t.\zeta_{ij}\, a_i^{\dagger}a_j + H.c.\right] \qquad (2)$$

Bond breaking in the system arises with probability W. Specifically, $t_{ij} = t.\zeta_{ij}$, where ζ_{ij} is a binary random variable:

$$\zeta_{ij} = \begin{cases} 1 & with\ probability\ 1-W, \\ 0 & with\ probability\ W \end{cases} \qquad (3)$$

We construct the Hamiltonian matrix with appropriate periodic boundary conditions having the off-diagonal bond breaking disorder and then perform the exact diagonalization.

Numerical results and discussions

To stimulate the Anderson transition, we perform exact diagonalization of the Anderson Hamiltonian (2) for an individual particle,

@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

where the eigenstates are established within a 3D lattice. In the following results, we consider three distinct scenarios: (a) zero disorder, resulting in eigenstates of Bloch waves. (b) finite (weak) disorder, which leads to the demonstration of mixed states, encompassing both extended and localized states. (c) infinite (strong) disorder, exclusively yielding localized states.

Density of states

The density of states (DOS) can be calculated analytically following [9]:

$$DOS\ \left(\rho(E)\right) = \frac{1}{2\pi}\frac{\partial k}{\partial E} \tag{4}$$

where $\vec{k} = (k_x, k_y, k_z)$.

In the case of zero disorder, one can easily find the energy dispersion for (2):

$$E = -2tcosk_x - 2tcosk_y - 2tcosk_z \tag{5}$$

and the energy band spans from $-6t < E < +6t$, and hence we define the band width as $BW = 12t$.

In fig.1, we present an insightful depiction of the profound impact of disorder on the DOS in the context of the 3D lattice. The figure illustrates the DOS results across a spectrum of disorder scenarios, encompassing the three extremes: zero disorder, weak disorder, and strong disorder. In fig we observe a distinct peak at $E = 0$, which becomes sharper as the disorder strength increases. In the absence of disorder, for a nearest-neighbour tight-binding model in the thermodynamic limit, there is a known singularity at the band edge. Introducing disorder eliminates this singularity at the band edge. For diagonal disorder, no such singularity appears in the DOS, unlike the case of off-diagonal disorder. In off-diagonal disorder, this singularity is linked to the delocalized nature of the wavefunction at the centre of the band.

@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

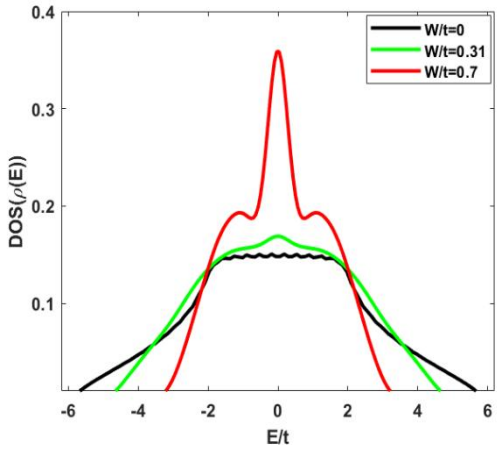


Fig. 1. DOS for different values of disorder. As the disorder increases, the peak at $E = 0$ becomes more pronounced.

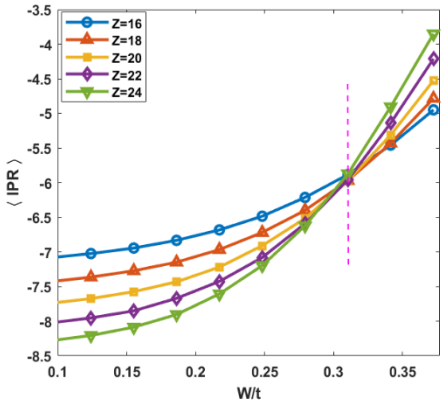


Fig. 2. IPR for different system sizes. Crossing of curves indicates to the mobility edge.

Inverse Participation Ratio and Mobility Edge In order to provide a broader perspective on the lattice depicted in fig.1, one can describe the eigenstates by employing the inverse participation ratio (IPR).

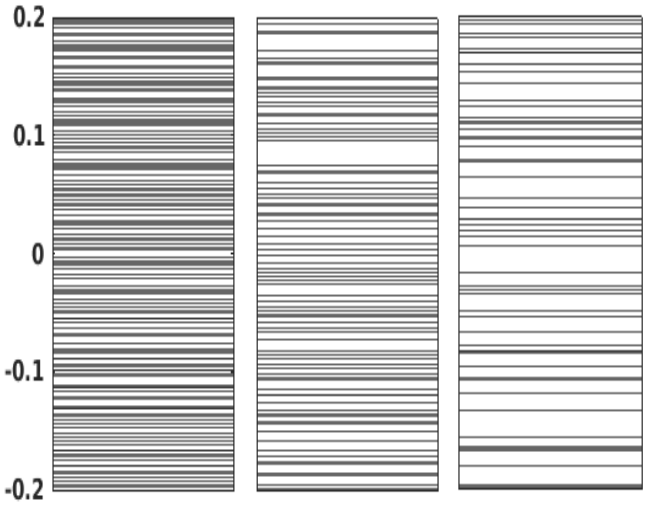
$$IPR = \sum_i |\psi(i)|^4 \tag{6}$$

@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

In fig.2. we compute IPR as a function of disorder W . Result of IPR provides confirmation that, in systems with mild disorder, the eigenstates spanning the entire energy band exhibit delocalization. As we approach the critical disorder threshold, the vertical dashed line, W_c , IPR increases significantly, illustrating the anticipated shift from a metallic state to an insulating state. Additionally, the numerical data indicates that localization begins to manifest even before reaching the critical disorder strength, $w < W_c$. In the context of AL, this critical threshold, $|E| < E_c$, represents a Metal-Insulator transition for a fixed disorder strength, and is referred as the mobility edge. In the system comprising noninteracting electrons with fermi energy, E_F lower than the mobility edge ($E_F < E_c$), the system behaves as an insulator. We have performed 3000 disorder realizations while computing IPR vs W.

Level statistics

Level statistics provides another important insight into the transport properties of disordered systems by analysing the eigen-energy spectrum. Fig.3 shows the eigen-energy spectrum for the metallic, critical, and insulating regimes. It is clear that the three spectra are qualitatively different. This difference can be quantified by studying the statistical distribution of the gaps between two neighbouring eigen-energies of the random Hamiltonian.



@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

Fig. 3. Eigen-energies of the disordered 3D lattice. The first plot(left), representing the metallic regime at weak disorder strength $W = 0.05$. The second plot(middle) corresponds to the critical regime at the disorder value $W = 0.3$. The third plot(right) illustrates the localized regime at a high disorder strength $W = 0.6$.

Figure illustrates that in the metallic regime (left), the energy levels are almost evenly spaced, indicating extended states and strong level repulsion due to delocalized wavefunctions. In the critical regime (middle), gaps begin to appear in the energy spectrum, reflecting the coexistence of extended and localized states as the system transitions toward localization. Finally, in the insulating regime (right), most of the energy levels correspond to localized states, resulting in a highly irregular spectrum with minimal level repulsion.

These distinctions in level statistics are quantified by studying the distribution of nearest-neighbour energy spacings. For metallic systems, the spacing follows the Wigner-Dyson distribution, characteristic of level repulsion. In contrast, in the insulating regime, the spacing distribution resembles a Poisson distribution, consistent with the random, uncorrelated nature of localized states. The critical regime displays a mixture of both behaviours, reflecting its intermediate nature between metallic and insulating phases.

Conclusion

We have studied Anderson localization in 3D disordered lattice within the tight-binding model where hopping's are restricted to nearest-neighbour sites. We have introduced off diagonal bond breaking disorder in the system to yield the Anderson transition. We have shown that the system undergoes the MI transition when the strength of the disorder increases over critical value. We study how disorder affects the energy spectrum and spatial distribution of electronic eigenstates in the insulating regime, as well as in the critical region of the MI transition. Since we concentrate on the one-electron propagation at zero temperature, no effects of electron-electron interaction and incoherent scattering are discussed in the paper.

References:

1. Abrahams, E., & PWA. (1979). D.C.L. and T.V.R. scaling theory of localization: Absence of quantum diffusion in two dimensions. *Physical Review Letters*, *42*,

@2025 International Council for Education Research and Training
ISSN: 2959-1376
2025, Vol. 04, Issue 02, 193-200
DOI: https://doi.org/10.59231/SARI7818

4. S. Aubry and G. Andr´e. Analyticity breaking and Anderson localization in incommensurate lattices. *Ann. Isr. Phys. Soc.3* **18**, (1980).

2. Anderson, P. W. (1958). Absence of diffusion in certain random lattices. *Phys. Rev. Reviews of Modern Physics* **50**, (1978), *109*, 2. N. F. Mott. Electrons in glass.

3. Ogwazu, J. E., & Ayannuga, O. M. (2024). Teachers' Integration Strategies and Challenges on inclusion in selected public primary schools in Lagos, Nigeria. *Edumania-An International Multidisciplinary Journal*, *02*(02), 175–192. https://doi.org/10.59231/edumania/9046

4. Chalker, J. T., Pickles, T. S., & Shukla, P. (2010). Anderson localization in tight-binding models with flat bands. *Physical Review. Part B*, *82*(10). https://doi.org/10.1103/PhysRevB.82.104209

5. Guan, C., & Guan, X. (2019). *A brief introduction to Anderson Localization*. Department of Phy, Massachusetts Institute of Technology.

6. Gupta, T. (2025c). Redefining Employment Relations: Understanding Recent Advances and Innovative ideas Guiding the New Era of human resource development. *Shodh Sari-An International Multidisciplinary Journal*, *04*(01), 95–110. https://doi.org/10.59231/sari7781

7. E. N. Economu. *Economou Green's Functions in Quantum Physics*. (1990).

8. Markos, P. (2006). Numerical analysis of the Anderson localization. *Acta Physica Slovaca*, 56.

9. Rodríguez, A. MA MD J. R. L. G. S. V. A. M. F. D. A. J. P. L. (2001). Absence of weak localization in two-dimensional disordered Frenkel lattices. *Journal of Luminescence*, *94*.

Received on Dec 23, 2024
Accepted on Feb 05, 2025
Published on April 01, 2025